hain nodes :
    10   11   12
ing nodes :
    1   2   3   4   5   6   7   8   9
hain bonds :
    4-10   5-12   10-11
ing bonds :
    1-2   1-5   2-3   2-7   3-4   3-6   4-5   6-9   7-8   8-9
xact/norm bonds :
    1-2   1-5   2-3   2-7   3-4   3-6   4-5   4-10   5-12   6-9   7-8   8-9
xact bonds :
    10-11

atch level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:CLASS   7:CLASS   8:CLASS   9:Atom   10:Atom
    11:Atom   12:Atom